Non-Ergodicity of the 1D Heisenberg Model

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Abstract

The relevance of zero-energy functions, coming from zero-energy modes and present in the structure of bosonic Green's functions, is often underestimated. Usually, their values are fixed by assuming the ergodicity of the dynamics, but it can be shown that this is not always correct. As the zero-energy functions are connected to fundamental response properties of the system under analysis (specific heat, compressibility, susceptibility, etc.), their correct determination is not an irrelevant issue. In this paper we present some results regarding the zero-energy functions for the Heisenberg chain of spin-1/2 with periodic boundary conditions as functions of the number of sites, temperature and magnetic field. Calculations are pursued for finite chains, using equations of motion, exact diagonalization and Lanczos technique, and the extrapolation to thermodynamic limit is studied.

Introduction The issue of ergodicity of physical systems is not new. A system is ergodic if it goes through every point of phase space during its time evolution. In such systems, the equilibrium averages (i.e., the time averages) are equal to the ensemble averages, which are much easier to compute. Anyway, we have to face the problem of non-ergodicity of many physical systems (e.g., the existence of even one integral of motion divides the phase space into separate subspaces not connected by the dynamics). The lack of ergodicity has measurable effects as the well-known difference between the static isolated (or Kubo [1]) susceptibility and the isothermal one [2, 3].

In the widely used formalism of Green's functions the issue of ergodicity appears as a difficulty in the determination of the zero-frequency functions present in the bosonic propagators [4]-[11]. The problem reappears also in e.g., composite operator method [12]. The equations of motion do not uniquely determine causal Green's functions and correlation functions but only up to some momentum function which severely affects the self-consistent calculation of the retarded Green's functions too. Usually, these zero-frequency functions are fixed by assigning them their ergodic values, but this can not be justified a priori. Wrong determination of them dramatically affects the values of directly measurable quantities like compressibility, specific heat, magnetic susceptibility. According to this, they should be calculated case by case.

In this paper, we calculate the zero-frequency functions for the Heisenberg chain of spin-1/2 and show that they take non-ergodic values for finite lengths and in the bulk limit too.

Definitions One of the main aims of condensed matter calculations is to compute the correlation functions of the physical system under analysis:

$$C(i,j) = \left\langle \psi(i)\psi^{\dagger}(j) \right\rangle \tag{1}$$

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where $i = (\mathbf{i}, t)$ stands for both spatial $\mathbf{i}$ and temporal t coordinates and ψ for any operator relevant to the dynamics under study. The Fourier transform in frequency of the correlation functions can be expressed in terms of the eigenstates $|n\rangle$ and eigenenergies E_n of the system in the following way

$$\begin{aligned} C(\mathbf{i},\mathbf{j},\omega) &= 2\pi\delta(\omega)\Gamma_{\psi\psi^\dagger}(\mathbf{i},\mathbf{j}) \\ &+ \frac{2\pi}{Z}\sum_{\substack{n,m \\ E_n\neq E_m}} \mathrm{e}^{-\beta E_n}\langle n|\psi(\mathbf{i})|m\rangle\langle m|\psi^\dagger(\mathbf{j})|n\rangle\delta\left[\omega+(E_n-E_m)\right] \end{aligned} \tag{2}$$

where the *zero-frequency function* $\Gamma_{\psi\psi^\dagger}(\mathbf{i},\mathbf{j})$ is defined as:

$$\Gamma_{\psi\psi^\dagger}(\mathbf{i},\mathbf{j}) = \frac{1}{Z}\sum_{\substack{n,m \\ E_n=E_m}} \mathrm{e}^{-\beta E_n}\langle n|\psi(\mathbf{i})|m\rangle\langle m|\psi^\dagger(\mathbf{j})|n\rangle \tag{3}$$

Its ergodic value is [1, 13]:

$$\Gamma^{erg}_{\psi\psi^\dagger}(\mathbf{i},\mathbf{j}) = \langle\psi(\mathbf{i})\rangle\langle\psi^\dagger(\mathbf{j})\rangle \tag{4}$$

In this manuscript, we focus on the Heisenberg chain of spin-1/2 with periodic boundary conditions in presence of an external magnetic field directed along z and proportional to h:

$$H = J\sum_{\mathbf{i}}\vec{S}(i)\vec{S}\left(i^\alpha\right) - h\sum_{\mathbf{i}}S^z(i) \tag{5}$$

where $i^\alpha = (\mathbf{i}+1, t)$, J is the exchange coupling and $\vec{S}(i)$ is the spin-1/2 operator at the site $\mathbf{i}$ of the chain of N sites.

Results We diagonalize exactly the Heisenberg model on three sites in magnetic field, obtaining eigenvalues and eigenvectors. Then, Eq. (3) yields the following functional dependence on temperature and magnetic field of the zero-frequency function $\Gamma_{S_zS_z}(\mathbf{i},\mathbf{j})$ (see Fig. 1):

$$\Gamma_{S_zS_z}(\mathbf{i},\mathbf{i}) = \frac{5}{36} + \frac{1-2\mathrm{e}^{\beta h}+\mathrm{e}^{2\beta h}}{9\left[1+\mathrm{e}^{2\beta h}+2\mathrm{e}^{\frac{3}{2}\beta J}\mathrm{e}^{\beta h}\right]} \tag{6}$$

$$\Gamma_{S_zS_z}(\mathbf{i},\mathbf{i}+1) = -\frac{1}{36} + \frac{5-4\mathrm{e}^{\beta h}+5\mathrm{e}^{2\beta h}}{18\left[1+\mathrm{e}^{2\beta h}+2\mathrm{e}^{\frac{3}{2}\beta J}\mathrm{e}^{\beta h}\right]} \tag{7}$$

We can see that the zero-frequency functions behave quite differently then their ergodic values $M^2 = \langle S_z\rangle^2$ and with a quite strong dependence on both magnetic field and temperature. According to this, a careful determination of them is absolutely necessary and we cannot rely at all on the ergodic values.

Let us now analyze the situation as function of the number N of sites. To perform calculations for chains with a number of sites greater than 4 it is necessary to use numerical tools like the exact diagonalization and the Lanczos method. The thermodynamic limit will be extrapolated by means of a $1/N$ analysis.

For zero temperature the ergodic value of the on-site zero-frequency functions $\Gamma_{S^+S^-}$ is always zero, not depending on the magnetic field; for the on-site $\Gamma_{S^zS^z}$ it is zero excluding three cases: 1) $J<0$ and finite magnetic field ($\Gamma^{erg}_{S^zS^z}=\frac{1}{4}$); 2) $J>0$ and high magnetic field $h\gg J$ ($\Gamma^{erg}_{S^zS^z}=\frac{1}{4}$); 3) $J>0$ and magnetic field with values corresponding to energy level crossing (for finite N; e.g., $h=3J/2$ for 3 sites).

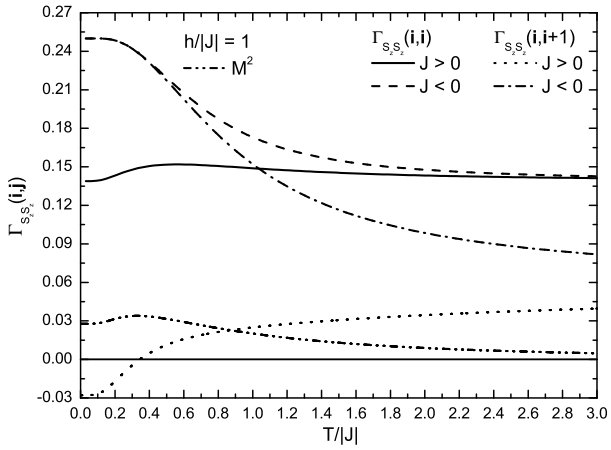

Figure 1: For the 3-site chain, the on-site and nearest-neighbor zero frequency functions, for antiferromagnetic ($J > 0$; solid line and dotted line, respectively) and ferromagnetic ($J < 0$; dashed and dot-dashed line, respectively) exchange coupling, together with squared magnetization M^2 (double dot-dashed line), at magnetic field $h/|J| = 1$, are plotted versus temperature

Properly calculated zero-frequency functions $\Gamma_{S^zS^z}$ and $\Gamma_{S^+S^-}$ behave differently. For $J < 0$, $T = 0$ and $h = 0$ both constants are non-zero; this is due to the degeneracy of the ground state coming from the fact that both S^z and S^+ are constants of motion and higher value of the total spin is selected. We also have the exact relation $\Gamma_{S^zS^z} = \frac{1}{2}\Gamma_{S^+S^-}$, which can be derived from the algebra in absence of magnetization. The inclusion of a non-zero magnetic field removes the degeneracy, by fixing the value of S^z and giving dynamics to S^+, and switches the functions to their ergodic values.

For $J > 0$, $T = 0$ and $h = 0$ both constants are zero or non-zero, depending whether the number of sites in the chain is even or odd, respectively. The relation $\Gamma_{S^zS^z} = \frac{1}{2}\Gamma_{S^+S^-}$ still holds as the magnetization is zero in this case too. The discrepancy with respect to the ergodic values for *o*dd chains is due to the impossibility to pair up all spins on selecting the lower value of the total spin: *e*ven chains have a unique $S^z = 0$ singlet-like ground state, the *o*dd ones have a degenerate $S^z = 1/2$ ground state. The inclusion of the magnetic field sets $\Gamma_{S^+S^-}$ again to zero (except for the values generating a level crossing and, consequently, a degeneracy), while $\Gamma_{S^zS^z}$ keeps its previous value or jumps to a higher one passing through level crossing values. As the magnetic field becomes high enough the system becomes fully polarized, the ground state is non-degenerate as for $J < 0$ and $h > 0$, and both constants set at their ergodic values.

These results were obtained solving numerically chains up to 25 sites, using exact diagonalization and Lanczos method. Now the main question: do these results hold also in the thermodynamic limit? In Fig. 2 we show the zero-frequency function $\Gamma_{S^zS^z}$ as a function of the inverse of the number of sites $1/N$ for $J > 0$ and $J < 0$, $T = 0$ and $h = 0$. For $J < 0$, $\Gamma_{S^zS^z}(\mathbf{i},\mathbf{j})$ is independent of the distance $|\mathbf{i}-\mathbf{j}|$ and is exactly given by $1/12+1/(6N)$ [14]. For $J > 0$, $\Gamma_{S^zS^z}(\mathbf{i},\mathbf{j})$ is a function of the distance $|\mathbf{i}-\mathbf{j}|$ and scales with N as shown in the figure (the lines represent very accurate fits). According to this, we have a non-ergodic behavior for

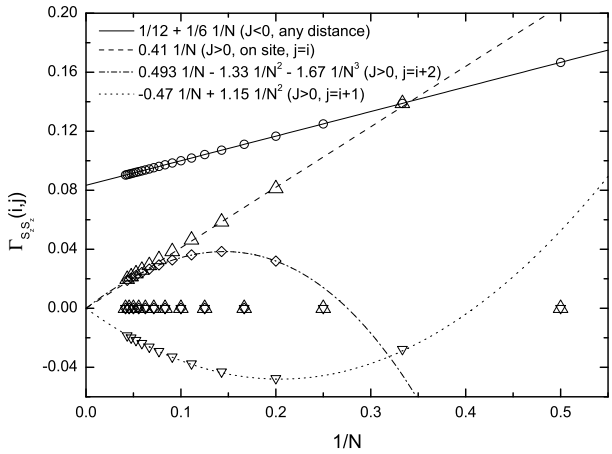

Figure 2: Zero-frequency functions for a N-site chain with ferromagnetic ($J < 0$; ◯) and antiferromagnetic ($J > 0$) coupling. In the latter case, zero-frequency functions are calculated on-site (△), for first (▽) and second neighbors (◇). The lines are fits of the numerical data, according to the formulae displayed in the legend

$J < 0$ which remains in the thermodynamic limit too. We wish to point out that this result is exact and must be taken into consideration by whoever needs to compute physical quantities like spin correlation functions and susceptibilities in the 1D Heisenberg model by means of analytical methods. $\Gamma_{S^zS^z}$ should be set to 1/12; any other value, the null ergodic one too, will induce wrong results and any approximation scheme not taking this into account, directly or self-consistently, will surely fail to reproduce the physical properties of the system. Non-ergodic behaviors for finite values of temperature and magnetic field cannot be excluded at all and are instead probable; we are performing numerical calculations in this direction and the results will be published elsewhere. Finally, it is worth noting that non-ergodic behaviors with a functional structure (i.e., zero-frequency functions with dependencies on temperature and magnetic fields as rich as those found for finite size chains) require the maximum attention in building up reliable conserving and/or self-consistent approximation scheme as any mistake in reproducing them will mine the possibility to comprehend the low-energy properties of the system.

References

[1] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).
[2] M. Suzuki, Progr. Theor. Phys. **43**, 882 (1970).
[3] M. Suzuki, Physica **51**, 277 (1971).
[4] K. W. H. Stevens and G. A. Tombs, Proc. Phys. Soc. **85**, 1307 (1965).
[5] J. F. Fernandez and H. A. Gersh, Proc. Phys. Soc. **91**, 505 (1967).
[6] H. Callen, R. H. Swendsen and R. Tahir - Kheli, Phys. Lett. **A 25**, 505 (1967).
[7] G. L. Lucas and G. Horwitz, J. Phys. A **2**, 503 (1969).
[8] T. Morita and S. Katsura, J. Phys. C **2**, 1030 (1969).
[9] P. C. Kwok and T. D. Schultz, J. Phys. C **2**, 1196 (1969).
[10] J. G. Ramos and A. A. Gomes, Il Nuovo Cimento **3 A**, 441 (1971).

[11] E. Fick and G. Sauermann, Quantum Statistics of Dynamic Processes, Springer-Verlag, New York, 1990.
[12] F. Mancini and A. Avella, cond-mat/0006377.
[13] D. Zubarev, Nonequilibrium Statistical Thermodynamics, Plenum, New York, 1974.
[14] In this specific case ($T = 0$, $h = 0$), the formula can be also exactly obtained by combinatorics.